NASA-TM-81440 19800009938

NASA Technical Memorandum 81440

INITIAL CHARACTERIZATION OF AN EXPERIMENTAL REFEREE BROADENED-SPECIFICATION (ERBS) AVIATION TURBINE FUEL

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January 1980

SUMMARY

Characterization data and a hydrocarbon compositional analysis are presented for a research test fuel designated as an Experimental Referee Broadened-Specification (ERBS) aviation turbine fuel. This research fuel, which is a special blend of kerosine and hydrotreated catalytic gas oil, is a hypothetical representation of a future fuel should it become necessary to broaden current kerojet specifications. It will be used as a reference fuel in research investigations into the effects of fuel property variations on the performance and durability of jet aircraft components, including combustors and fuel systems.

INTRODUCTION

Until recently there has been an abundance of mid-distillates from petroleum available for jet fuel. Demand for jet fuel is increasing at a time when there is severe competition for the available mid-distillates. A relaxation in property specifications for future jet fuels could minimize potential curtailments in supplies and might also lower costs. These future jet fuels may have higher aromatic content, higher freezing point, lower fuel volatility, higher viscosity, and poorer thermal stability. Presently a fuels data bank compiled by the Department of Energy (DOE) has shown a trend of increasing aromatics in jet fuels (ref. 1). Assessing the effect of changes in jet fuel properties and developing technology to use the fuels will require a large effort in combustor and engine testing. Such an effort is in progress at both NASA's Lewis Research Center and Wright-Patterson Air Force Base.

Requirements for an Experimental Referee Broadened-Specification (ERBS) aviation turbine fuel were proposed at a workshop held at Lewis in 1977 (ref. 2). They were written to avoid redundancy, to make it reasonably easy to supply the fuel, and to give sufficiently reproducible combustion characteristics. These specifications for a research fuel reflect the opinions of the subject workshop on what a future broad-property fuel might be like. They are subject to change as a better understanding of future feedstocks, processes, and product demand is obtained. However, for the present, a fuel with the proposed properties will serve as a reference or baseline fuel in research investigations into the effects of fuel property variations on the performance and durability of jet aircraft components, including combustors and fuel systems. A technical panel sponsored by the Coordinating Research Council (CRC) (ref. 3) recommended some slight modifications to the property requirements. The requirements

for the Experimental Referee Broadened-Specification aviation turbine fuel as suggested by CRC are given in table I. Other experimental fuels of lower quality could be blends of this fuel with a suitable blending stock.

This report gives the measured characteristics of the first acquisition of the ERBS fuel proposed in reference 2. Blend composition is discussed so that future acquisitions can preserve the "reference" characteristics of this fuel.

ERBS FUEL BLEND

The best method of obtaining ERBS fuel is directly from one stream of a refinery. For this to occur is unlikely because refineries usually do not operate on a fixed crude or crude blend. The next best method would be a blend of two refinery streams. Attempts to blend the fuel with only two refinery streams showed that the freezing point and flash point specifications could not be readily achieved. The CRC recommended that the flash point be modified from $100^{\circ} \pm 10^{\circ}$ F to 38° C (100° F) minimum and that the freezing point be increased from -20° F to -23° C (-10° F) maximum. These changes will not significantly affect the combustion characteristics of the fuel but will slightly affect ignition, altitude relight, and low-temperature behavior.

The kerosine and hydrotreated catalytic gas oil (HCGO) streams at the Marcus Hook refinery of the Sun Company were identified as suitable for blending ERBS fuel to table I requirements. A mixture of about 65 percent kerosine and 35 percent HCGO is required to blend ERBS fuel. Hydrogen content was the controlling factor in determining blend composition. Sample blends made at different times met the requirements; however, the sample blends showed that care must be taken to meet the freezing-point specification. The available range of hydrogen content should be sufficient for adjusting the blend to meet the freezing point specification.

An antioxidant additive and long-term storage under a blanket of gaseous nitrogen are required for this fuel blend. The antioxidant to be used is an alkylated phenol specified in ASTM D-1655. The ERBS fuel analyzed for this report had no antioxidant.

ERBS FUEL CHARACTERIZATION

The test results of, the fuel requirements for, and the analytical techniques used to characterize the initial acquisition of 600 barrels of ERBS fuel are summarized in table I. Several of the test methods were revised from those originally specified; the revised methods include those for determining sulfur as mercaptan, total nitrogen, naphthalenes, the hydrocarbon compositional analysis, and the distillation temperatures.

The weight percentage of mercaptan sulfur was determined by using the potentiometric method (ASTM D-3227) rather than the color-indicator method (ASTM D-1219), since the latter has been discontinued. The total weight percentage of nitrogen was determined by the combustor-microcoulometric method (ASTM D-3431) as a well-characterized alternative to the Kjeldahl method.

Because of the relatively high concentration of naphthalenes in the fuel, ASTM method D-1840 was slightly modified. The accuracy of the reported result is somewhat in question because of the 328° C (622° F) final boiling point of the fuel. There is some indication from mass spectrographic data that the 13.2 percent by volume (15.7 percent by weight) naphthalene content reported had been elevated by the presence of interfering compounds. The hydrocarbon compositional analysis was performed by group separation before instrumental analyses rather than by gas chromatography - mass spectrometry (GCMS) as originally specified in reference 2. The separation was performed by using a modification of the fluorescent indicator adsorption method (ASTM D-1319) followed by gas chromatographic and mass spectrographic analyses of the alkane (saturate) fraction and by mass spectrographic and nuclear magnetic resonance analyses of the aromatic fraction. The results are presented in table II. The loss reported in table II(a) is primarily due to the more volatile components of the alkane (saturate) fraction. Tables II(b) to (d) give the composition of the ERBS fuel and should serve as a "fingerprint" for the fuel. Subsequent ERBS fuel blends should not vary significantly from this composition.

The standard method for distilling petroleum products (ASTM D-86) was sufficient to characterize the fuel and therefore was used instead of the standard method for distilling crude petroleum (ASTM D-2892). The distillation curve is shown in figure 1, and selected distillation data are presented in table I.

A series of five trials at various temperatures between 237.5° and 260° C (460° and 500° F) were used to determine the ERBS fuel breakpoint temperature. A plot of the results, figure 2, shows that the breakpoint temperature is at approximately 256° C (483° F) if the breakpoint condition is defined by a spun TDR of 13 or by a test-filter pressure drop of 25 mm Hg. No pressure drop was observed in any of the five trials.

The results of a selective elemental analysis by arc emission spectroscopy are presented in table III. Sample treatment included ashing, dissolving the residue in a solution of hydrochloric and nitric acid, and quantitatively spiking graphite electrodes with the resulting solution. The accuracy of the analysis is approximately ±50 percent of the values reported. Those elements that were not detected are reported as "less than" the method detection limits for the sample. The uncharacteristically high concentration of lead was verified by atomic absorption spectroscopy but is believed to originate from the storage container rather than from the ERBS fuel itself.

CONCLUDING REMARKS

A source for ERBS aviation turbine fuel has been identified as a blend of the kerosine and hydrotreated catalytic gas oil (HCGO) streams from the Marcus Hook refinery of the Sun Company. The blend is about 65 percent kerosine and 35 percent HCGO. The freezing point specification is the most difficult to meet; however, the available range for hydrogen content is sufficient for adjusting the blend to freezing point specifications. The results of inspection data, including hydrocarbon compositional analysis and metals analysis, are presented.

REFERENCES

1. Shelton, E. M.: Aviation Turbine Fuels, 1978. BETC/PPS-79/2, U.S. Department of Energy, 1979.

2. Longwell, J. P., ed.: Jet Aircraft Hydrocarbon Fuels Technology. NASA CP-2033, 1977.

3. Coordinating Research Council Annual Report for Year Ending June 30, 1979, Coordinating Research Council, Inc., Atlanta, Ga., p. 45.

TABLE I. - EXPERIMENTAL REFEREE BROADENED-SPECIFICATION (ERBS) AVIATION TURBINE FUEL - REQUIREMENTS AND BLEND RESULTS

Property	Blend results	Requirements	Test method
Composition:			
Hydrogen, wt %	12.86	12.8±0.2	NMR
Atomatics, vol %	35.0	Report	ASTM D-1319
Sulfur, mercaptan, wt %	0.0005	0.003 max.	ASTM D-3227
Sulfur, total, wt %	0.085	0.3 max.	ASTM D-1266
Nitrogen, total, wt %	0.0054	Report	ASTM D-3431
Naphthalenes, vol. %	13.2	Report	ASTM D-1840
Hydrocarbon compositional analysis	Table II	Report	GCMS[a]
Volatility:			
Distillation temperature, °C (°F)			
Initial boiling point	162 (324)	Report	ASTM D-86
10 Percent	188 (370)	204 (400) max.	↓
50 Percent	215 (419)	Report	↓
90 Percent	279 (534)	260 (500) min.	↓
Final boiling point	328 (622)	Report	↓
Residue, percent	1.2	Report	↓
Loss, percent	0.3	Report	↓
Flash point, °C (°F)	60 (140)	[b]38 (100) min.	ASTM D-56
Gravity, API (15° C)	37.1	Report	ASTM D-287
Gravity, specific (15°/15° C)	0.8381	Report	ASTM D-1298
Fluidity:			
Freezing point, °C (°F)	-29 (-20)	[b]-23 (-10) max.	ASTM D-2386
Viscosity, at -23° C (-10° F), cS	7.2	12 max.	ASTM D-445
Net heat of combustion, kJ/kg (Btu/lb)	42 427 (18 275)	Report	ASTM D-2382
thermal stability:			
JFTOT, breakpoint temperature, °C (°F) (TDR, 13; and ΔP, 25 mm Hg)	255.5 (492)	238 (460) min.	ASTM D-3241

[a]For this paper, test method was FIA spearation followed by group analysis.
[b]Modified from that in ref. 2.

TABLE II. - HYDROCARBON COMPOSITIONAL ANALYSIS RESULTS

(a) Modified FIA separation by ASTM D-1319, in wt %

Aromatics	34.3
Saturates	60.8
Olefins	0.0
Loss	4.9

(b) Normal paraffins in fuel by gas chromatography, in wt %

C_9	0.67	C_{15}	0.73
C_{10}	2.07	C_{16}	0.61
C_{11}	2.68	C_{17}	0.55
C_{12}	2.43	C_{18}	0.36
C_{13}	1.64	C_{19}	0.18
C_{14}	0.85	C_{20}	0.12

(c) Mass spectrometric group analysis by ASTM D-2425, in wt %

Saturate group		Aromatic group	
Paraffins	37.1	Paraffins	0.6
Noncondensed cycloparaffins	17.7	Cycloparaffins	1.9
Condensed dicycloparaffins	4.7	Alkybenzenes	10.8
Condensed tricycloparaffins	1.0	Indanes and tetralins	5.6
Alkybenzenes	0.3	Indenes and $C_N H_{(2N-10)}$	0.3
		Naphthalenes	0.0
		Alkynaphthalenes	9.5
		Benzothiophenes	0.4
		Acenaphthenes	2.6
		Fluorene	1.3
		Triaromatics	1.4

(d) Nuclear magnetic resonance of aromatic fraction

Average molecular weight	190.2
Average molecular formula	$C_{14.5}H_{16.3}$
Aromaticity	0.62
Aromatic rings per molecule	1.7
Aromatic ring carbons per molecule	8.9
Saturate carbon content, percent	38.2
Alkyl substituents per molecule	3.1
Carbons per alkyl substituent	1.8
Carbon-hydrogen ratio of alkyl groups	5.55
Naphthenic carbon content, percent	6.7
Naphthene rings per molecule	0.3
Naphthene rings per substituent	0.1
Nonbridge aromatic ring carbon content, percent	51.7
Nonbridge aromatic carbons per molecule	7.5
Substitution of nonbridge aromatic carbons, percent	43.2
Monoaromatic content, percent	38.3
Diaromatic content, percent	49.8
Triaromatic content, percent	11.9

TABLE III. - ELEMENTAL ANALYSIS

BY ARC EMISSION SPECTROSCOPY

Element	Concentration, ppm
Al	0.0005
As	<0.003
Ca	0.001
Cd	<0.0004
Cr	<0.0001
Cu	0.01
Fe	0.002
Mg	0.0002
Mn	<0.0003
Mo	0.001
Na	0.003
Ni	0.002
P	<0.01
Pb	0.08 ([a]0.12)
Si	0.02
Sn	0.001
Ti	<0.0003
V	0.0008
Zn	0.001

[a]Value determined by atomic absorption spectroscopy.

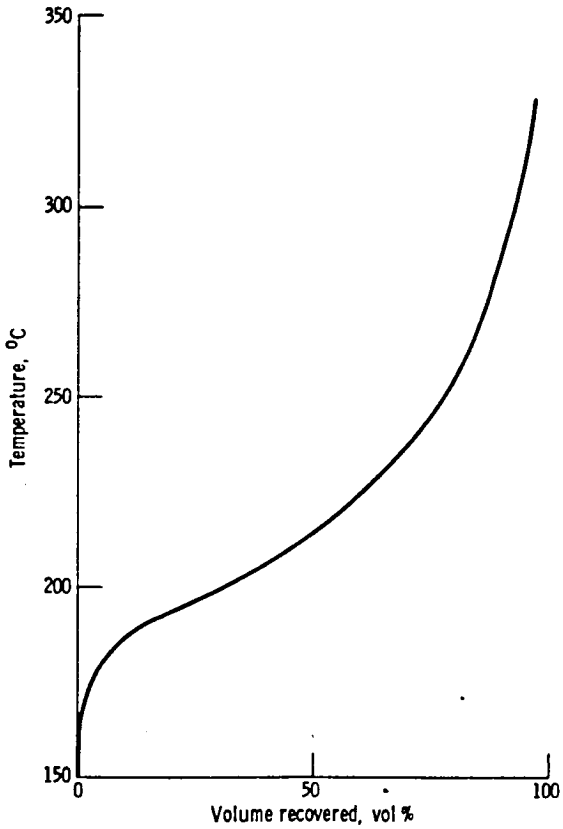

Figure 1. - D-86 distillation curve.

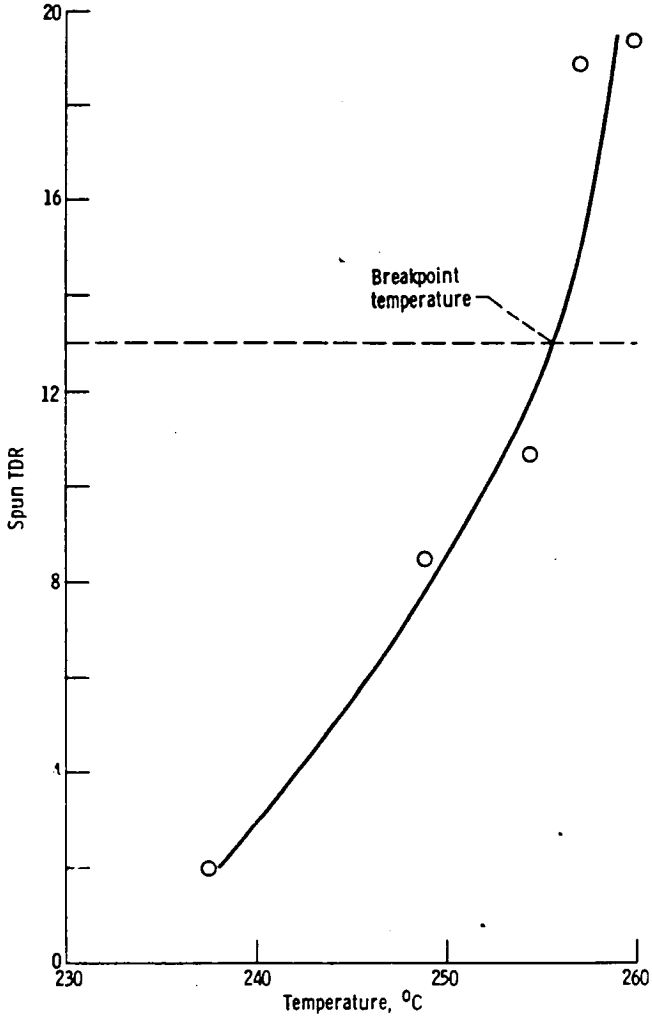

Figure 2. - JFTOT breakpoint determination.

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA TM-81440		

4. Title and Subtitle	5. Report Date
INITIAL CHARACTERIZATION OF AN EXPERIMENTAL REFEREE BROADENED-SPECIFICATION (ERBS) AVIATION TURBINE FUEL	January 1980
	6. Performing Organization Code
7. Author(s)	8. Performing Organization Report No.
George M. Prok and Gary T. Seng	E-206
	10. Work Unit No.
9. Performing Organization Name and Address	
National Aeronautics and Space Administration Lewis Research Center Cleveland, Ohio 44135	11. Contract or Grant No.
	13. Type of Report and Period Covered
12. Sponsoring Agency Name and Address	Technical Memorandum
National Aeronautics and Space Administration Washington, D.C. 20546	14. Sponsoring Agency Code

15. Supplementary Notes

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17. Key Words (Suggested by Author(s))	18. Distribution Statement
Fuels Jet engines Combustion	Unclassified - unlimited STAR Category 28

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price*
Unclassified	Unclassified		

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